Supplementary Materials

MSstatsQC: Longitudinal system suitability monitoring and quality control for targeted proteomic experiments

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Running Title: MSstatsQC - Statistical Process Control

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1. Monitoring algorithms and implementation

All algorithms are implemented in the R package and a Shiny application.

- Related materials and links are available through www.msstats.org/msstatsqc.

- R package is available at https://github.com/srtaheri/MSstatsQC

- Shiny application can be reached through https://eralpdogu.shinyapps.io/msstatsqc/ or using RunShiny() function in the R package. Source code is available at https://github.com/srtaheri/msstats-qc.

2. Results for simulated datasets

Supplementary Figure 1: **Results for simulated data: detecting isolated outliers with control charts.** A, CUSUMm chart of a representative peptide (VYVEELKPTPEGDLEILLQK) across the study. B, CUSUMv chart of a representative peptide (VYVEELKPTPEGDLEILLQK) across the study.
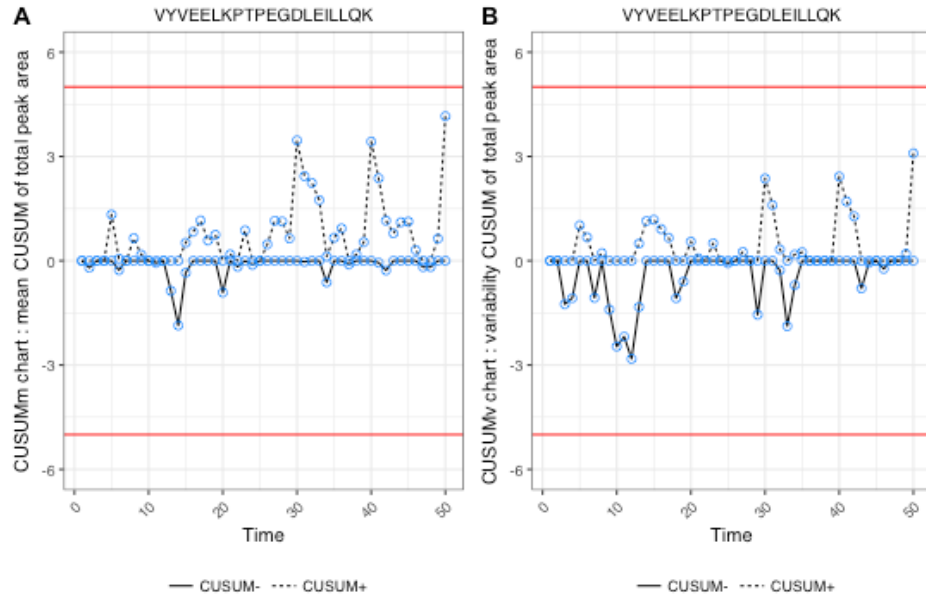
Supplementary Figure 2: **Results for simulated data: detecting a step shift with control charts.** Change point plot for mean of the integrated peak areas of a representative peptide (VYVEELKPTPEGDLEILLQK) across the study.
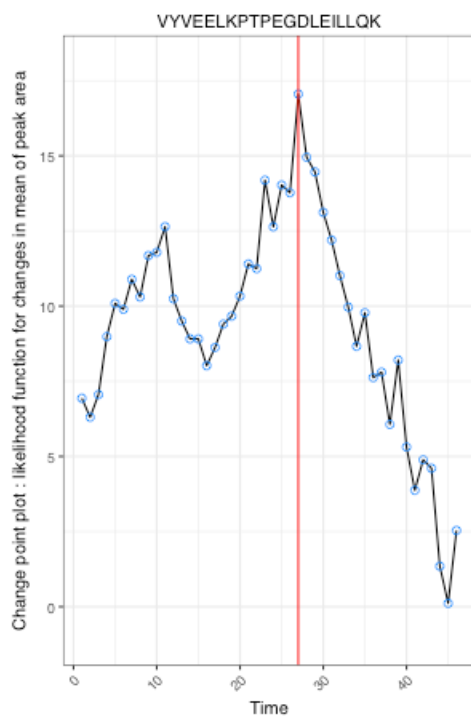
Supplementary Figure 3: **Results for simulated data: detecting a linear drift with control charts.** Change point plot for mean of the integrated peak areas of a representative peptide (VYVEELKPTPEGDLEILLQK) across the study.
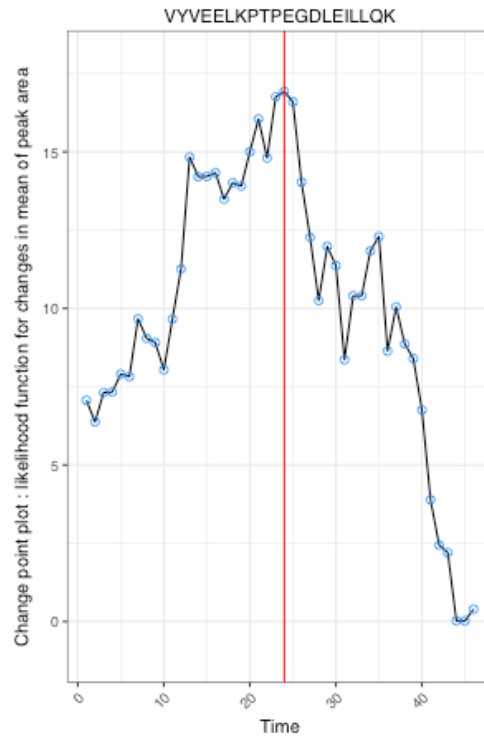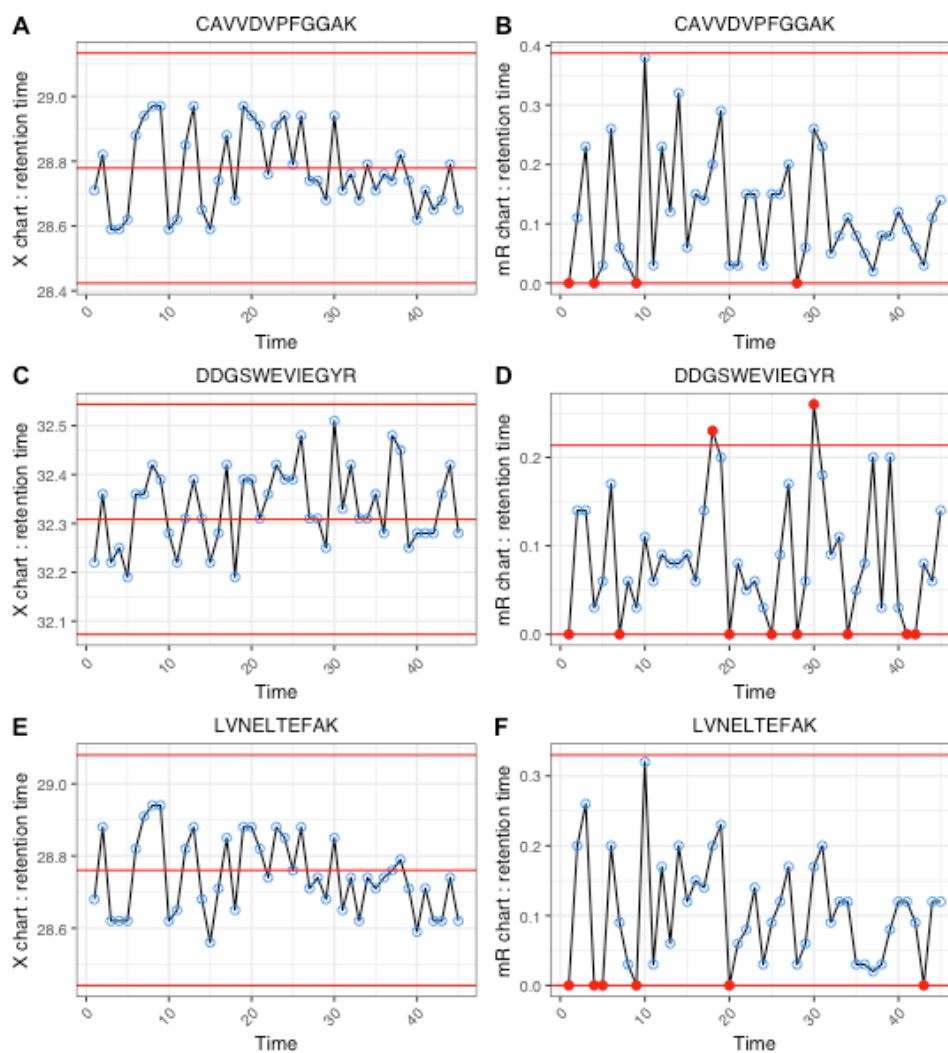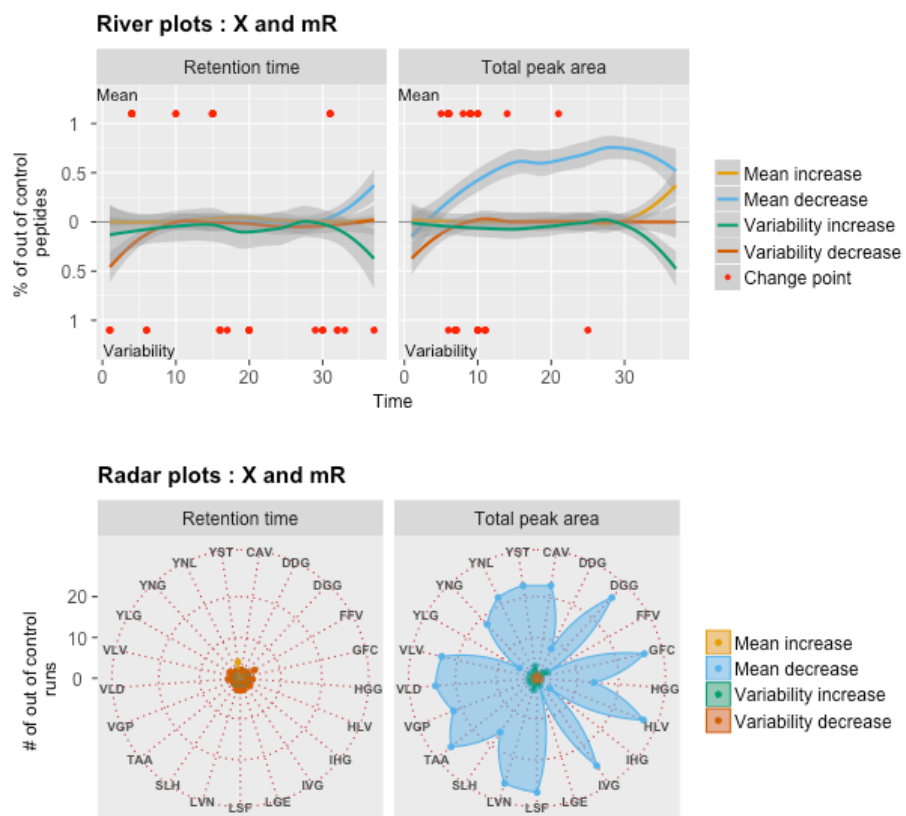
3. Results for CPTAC study 9.1

Supplementary Figure 4: **Importance of monitoring multiple peptides: Skyline output for CPTAC study 9.1 site 54.** Chromatography, peak area plot and retention time plot were generated for FFVAPFPEVFGK.
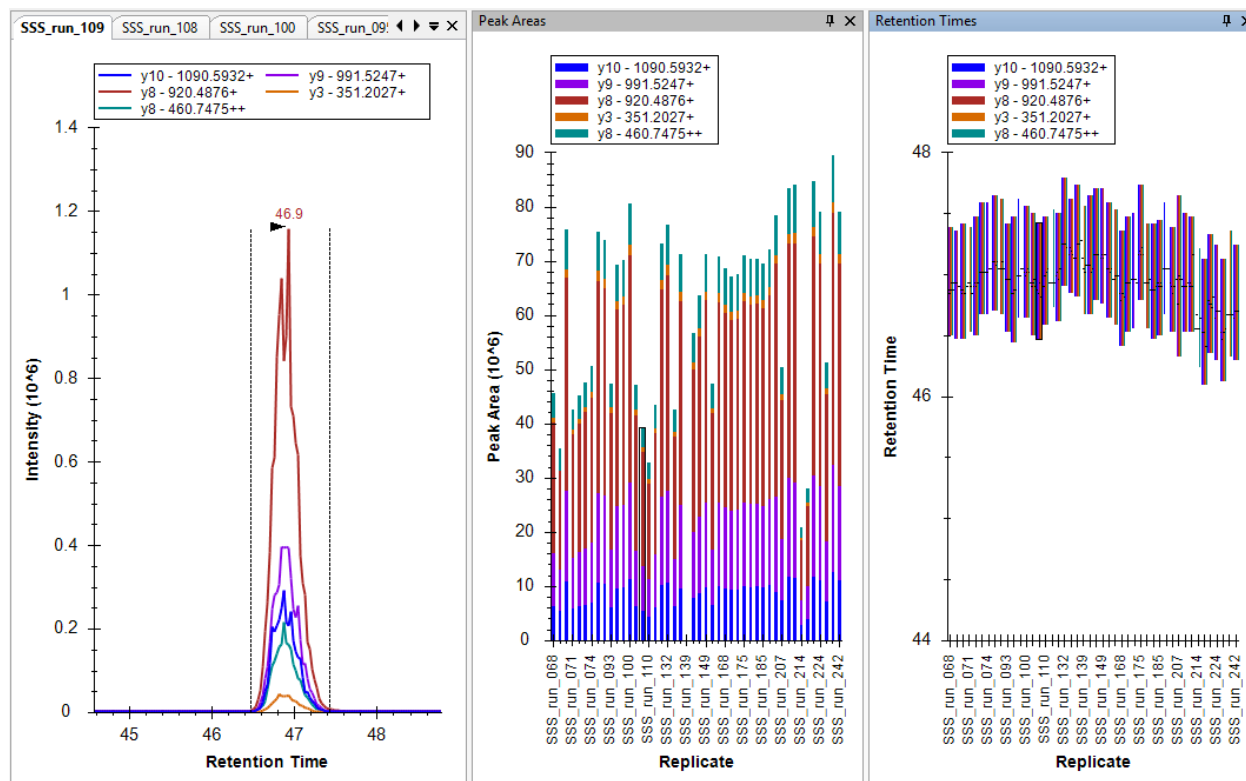
Supplementary Figure 5: **Importance of monitoring multiple peptides: XmR control charts (retention time) for CPTAC study 9.1 site 54.** A, X chart of CAVVDVPFGGAK. B, mR chart of CAVVDVPFGGAK. C, X chart of DDGSWEVIEGRYR. D, mR chart of DDGSWEVIEGRYR. E, X chart of LVNELTEFAK. F, mR chart of LVNELTEFAK.

Supplementary Figure 6: **Monitoring retention time and peak area: river and radar plots for CPTAC study 9.1 site 65.** A, river plot for XmR results. B, radar plot for XmR results.

Supplementary Figure 7: **Skyline output for CPTAC study 9.1 site 86.** Chromatography, peak area plot and retention time plot are generated for LVNELTEFAK.